

Tetrachlorophthalic acid
632-58-6 | DTXSID6060896

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 309 °C

Global applicability domain: Outside

Local applicability domain index: 1.80e-01

Confidence level: 5.02e-01

Nearest Neighbors from the Training Set

Image not found

Octanedioic acid

Measured: 346

Predicted: 332

Image not found

3-Ethyl-3-methylglutaric acid

Measured: 261

Predicted: 286

Image not found

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

Image not found

Heptanedioic acid

Measured: 342

Predicted: 332

Image not found

Benzoic acid, 2-phenoxy-

Measured: 355

Predicted: 325